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Quantum computer on a class of one-dimensional Ising systems

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Abstract

We discuss the problem of designing a quantum computer based on one-dimensional "alternating" Ising systems (linear chains with periodically recurring spin groups) in an external magnetic field which exceeds the interaction between spins. Loading and processing of information in the alternating Ising system may be accomplished by using a scheme suggested recently by Lloyd for heteropolymer systems. The detailed operation of a simple quantum logical device is described in the framework of a binary Ising system. Estimates of physical parameters are presented that show that the experimental realization of such quantum computer elements would be feasible as a research task. However, many difficulties remain to be addressed, before the approach discussed here would be applicable in real devices.

1. Introduction

The problem of the size limit of a bit of information is important, both from the fundamental point of view and also for computer miniaturization. Recently this problem has attracted additional attention because the current development of nanotechnology and design of semiconductor and metal devices is approaching the quantum size limit. Consequently, the idea of quantum computers in which the elements that carry bits of information are atoms has attracted the attention of many scientists [1–10]. Recently a scheme of driving a quantum computer with a sequence of laser pulses has been suggested [11]. We consider in this paper a class of systems (magnetic one-dimensional alternating Ising systems) which could be used as a base for future quantum computations. Using the idea suggested in Ref. [11] also we estimate the design parameters needed to implement this idea for a quantum computer on the alternating Ising systems.

It is usually assumed that the minimal system for carrying a bit of information is an atom with two states. The atom can be populated either in the ground state, or in the excited state. Information can then be represented by a set of atoms, some of which are in the ground state $|0\rangle$, and others in the excited state $|1\rangle$.

A computer is a set of elements, in which a bit of information can be transferred from one element to another. Each element should perform logical operations – for example, in the operation "not", zero

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transfers to one, and one transfers to zero. To create a computer, it is enough to use three main elements (operations), for example: "not", "controlled not", and "controlled controlled not" [1,2]. The controlled not has two inputs: a, a', and two outputs: b, b'. The parameter a' coincides with a, and a is the controlled parameter: if $a=1$, then $b'=$"not b", otherwise $b'=b$ (see Fig. 1). The controlled controlled not has three lines: $a, b, c \to a', b', c'$. Here $a'=a$, $b'=b$, $c'=$"not c", if $a=b=1$, otherwise $c'=c$. These three elements are enough to design an universal computer [1,2].

It is known that a chain of two-level atoms could in principal perform these logical operations [1]. The idea of quantum-mechanical computers has been discussed for many years (see, for example, Refs. [3–8]). In these previous discussions, the problems of constructing a Hamiltonian which describes the logical operations and the thermodynamics of computational processes has been investigated from various points of view. Many of these works were stimulated by results of Landauer [9] who showed that only irreversible logical operations require dissipation, and Bennett [10], who showed that dissipation of free energy is absent in the process of computation if one does not use irreversible elements. In fact, all elements that were discussed in the references above are reversible ones.

A new step in the discussion of quantum computers was made recently in the work of Lloyd [11], in which a quantum computer scheme is suggested involving an array of weakly coupled atoms. For computation one applies to the array a sequence of electromagnetic pulses. Ref. [11] considers a one-dimensional array of three types of two-level atoms (heteropolymer) ABC ABC ABC..., in which each atom possesses a long-lived excited state, and the resonant frequencies ω^{A}, ω^{B} and ω^{C} are different. The light pulses have the form of π-pulses, and transfer the atom from the ground state $|0\rangle$ to the excited state $|1\rangle$, or vice versa, from $|1\rangle$ to $|0\rangle$. The system is assumed to have only nearest-neighbor interaction, which shifts the energy levels of each atom as a function of the states of its neighbors. This means that each energy level splits into four levels. For example, instead of frequency ω^{A} one has four frequencies ω^{A}_{00}, ω^{A}_{01}, ω^{A}_{10}, ω^{A}_{11}, where ω^{A}_{ik} means that the left neighbor (C) is in the state $|i\rangle$, and the right neighbor (B) is in the state $|k\rangle$. So, we have twelve different frequencies for each complex ABC, as the resonant frequency of each atom depends on the states of its neighbors. It is supposed that all twelve frequencies are sufficiently different to be distinguished, and that the corresponding atoms can be driven selectively. So, the resonant pulse updates the states of all units of a given type as a function of its previous state and the states of the neighbors. For example, the pulse with frequency ω^{A}_{01} acts only on the atoms A_{01} (where subscript 01 denotes that left neighbors of atoms A are in the state $|0\rangle$, and right neighbors are in the state $|1\rangle$), and transfers atoms A from the state $|0\rangle$ to the state $|1\rangle$, or from $|1\rangle$ to $|0\rangle$.

It is shown in Ref. [11] that different sequences of resonant pulses permit one to load information, to process it, and to read-out the information. These possibilities are based on the properties of the edge atoms, whose frequencies are different from the frequencies of all other atoms. Consequently, one loads the information onto the edge atom of the array. To move information along the array one can use sequences of the type

$$\omega^{A}_{01}\omega^{A}_{11}\omega^{B}_{10}\omega^{B}_{11}\omega^{A}_{01}\omega^{A}_{11}\,. \tag{1.1}$$

The result of such a sequence of pulses is shown in Fig. 2, where we present all possible initial states of the neighboring atoms A and B. It is seen that the first pair of pulses changes the states of A atoms that have right neighbors in the excited state independently of the states of the left neighbors. The second pair of pulses changes the states of B atoms that have

a	0	0	1	1
b	0	1	0	1
a'	0	0	1	1
b'	0	1	1	0

Fig. 1. "Controlled not": $a'=a$; if $a=0$, $b'=b$; otherwise $b'=$not b.

	AB	$A^{*}B$	AB^{*}	$A^{*}B^{*}$
$\omega^{A}_{01}\omega^{A}_{11}$	AB	$A^{*}B$	$A^{*}B^{*}$	AB^{*}
$\omega^{B}_{10}\omega^{B}_{11}$	AB	$A^{*}B^{*}$	$A^{*}B$	AB^{*}
$\omega^{A}_{01}\omega^{A}_{11}$	AB	AB^{*}	$A^{*}B$	$A^{*}B^{*}$

Fig. 2. Change of the initial states of two neighbouring atoms A and B under the influence of the sequence (1.1). Asterisk means that an atom is in the excited state.

their left neighbors in the excited state. Finally, the third pair of pulses repeats the action of the first pair. As a result, we have an exchange of one information bit between the A and B atoms. Note that to move information from (or to) the edge atom one has to use pulses with the frequency of the edge atom. For example, if the edge atom is the A atom, to move information to the next atom B one should use the sequence $\omega_1^{\mathrm{A}}\omega_{10}^{\mathrm{B}}\omega_{11}^{\mathrm{B}}\omega_1^{\mathrm{A}}$, where ω_1^{A} is the frequency of the first atom when its neighbor is in the excited state.

As an example of processing the information in Ref. [11] a scheme is considered that is based on the modified sequence (1.1),

$$\omega_{01}^{\mathrm{A}}\omega_{11}^{\mathrm{A}}\omega_{11}^{\mathrm{B}}\omega_{01}^{\mathrm{A}}\omega_{11}^{\mathrm{A}}\,, \tag{1.2}$$

which differs from (1.1) by the absence of a pulse with frequency ω_{10}^{B}. If in the complex ABC the atom C is in the excited state, the result of (1.2) coincides with the result of (1.1). If the atom C is in the ground state, the pulse ω_{11}^{B} does not act on atom B, and the result of the action of the sequence (1.2) on the neighboring atoms A and B, in fact, coincides with the results of action on these atoms of the sequence $\omega_{01}^{\mathrm{A}}\omega_{11}^{\mathrm{A}}\omega_{01}^{\mathrm{A}}\omega_{11}^{\mathrm{A}}$, that does not change the states of A atoms. So, the sequence (1.2) changes the states of the neighboring atoms A and B if and only if the atom C is in the excited state. This result is known as the Fredkin gate on the triple ABC, with C as a control bit [12].

To read-out the information it is suggested in Ref. [11] to use more complicated systems, namely systems with an additional excited state $|2\rangle$ that decays quickly to the ground state $|0\rangle$. To read-out the value of a bit one moves this bit to the end of the chain, and applies a π-pulse that drives the transition between the states $|1\rangle$ and $|2\rangle$ of the edge atom. If the edge atom is in the excited state, then it will emit a photon whose frequency corresponds to the transition between levels $|0\rangle$ and $|2\rangle$. In contrast to the previous scheme, this one is irreversible and, consequently, dissipative because it involves spontaneous emission. Because of low photon detection efficiencies, one has to use several copies of a bit. Later Lloyd suggested a reversible scheme to read-out the information using two π-pulses [13]. According to this scheme if, for example, the edge atom is an A atom, one applies a sequence $\omega_1^{\mathrm{A}}\omega_0^{\mathrm{A}}$. If either of these pulses is attenuated, the edge atom is the ground state; if either of the pulses is amplified, then the edge atom is in the excited state. Another irreversible dissipative process appears in Ref. [11] in consideration of error correction. The error correction considerations in Ref. [11] also require use of the more complicated three-level system.

2. One-dimensional Ising systems

The first question of quantum computation is the choice of an appropriate system that can be realized as an actual device. In this paper we suggest quantum computations using one-dimensional Ising systems described by the Hamiltonian

$$\hat{H}=-\tfrac{1}{2}\sum_i\left(\omega\hat{\sigma}_i^z+J\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z\right)\,,\quad \hbar=1\,, \tag{2.1}$$

where σ_i^z is the Pauli operator, J is the effective constant of interaction which can be positive or negative, and ω is the resonant frequency for the effective spin when the interaction is absent. We can apply Lloyd's schemes for loading and processing of information if we consider a modified one-dimensional Ising system with three inequivalent effective spins. In this case, we have

$$\hat{H}=-\tfrac{1}{2}\sum_i\left(\omega_i\hat{\sigma}_i^z+J_{i,i+1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z\right)\,, \tag{2.2}$$

where the frequency ω_i takes three values ω^{A}, ω^{B}, and ω^{C}. The constant of interaction $J_{i,i+1}$ also takes three values that correspond to the interaction between effective spins AB, BC, and CA.

The eigenfunctions of the Hamiltonian (2.2) represent spin states of the type $|00111011\ldots\rangle$, i.e. some of the spins are in the ground state, and the rest are in the excited state. For example, if in some state of the system the spin B is in the ground state $|0\rangle$, and in another state this spin B occupies the level $|1\rangle$, and all other spins are unchanged, then the difference ΔE between the energies of these two states is

$$\Delta E=\omega^{\mathrm{B}}\pm J^{\mathrm{AB}}\pm J^{\mathrm{BC}}\,, \tag{2.3}$$

where the upper $(+)$ sign at J^{AB} corresponds to the state $|0\rangle$ of the neighboring spin A, and the lower $(-)$ sign at J^{AB} corresponds to the state $|1\rangle$ of this spin (the same is true for the sign at J^{BC} and spin C). So, we find the following four eigenfrequencies of the

Hamiltonian (2.2) which correspond to inversion of one spin B,

$$\omega_{00}^{B}=\omega^{B}+J^{AB}+J^{BC}, \quad \omega_{01}^{B}=\omega^{B}+J^{AB}-J^{BC},$$
$$\omega_{10}^{B}=\omega^{B}-J^{AB}+J^{BC}, \quad \omega_{11}^{B}=\omega^{B}-J^{AB}-J^{BC}. \tag{2.4}$$

Note that all these frequencies are multiply degenerate. There are analogous expressions for ω_{ik}^{A} and ω_{ik}^{C}. We emphasize that the Ising Hamiltonian (2.2) does not have off-diagonal terms. Consequently, there is no "band problem" for the Ising system. This simplifies quantum computer considerations for the Ising system, compared to those for the heteropolymer chain considered in Ref. [11].

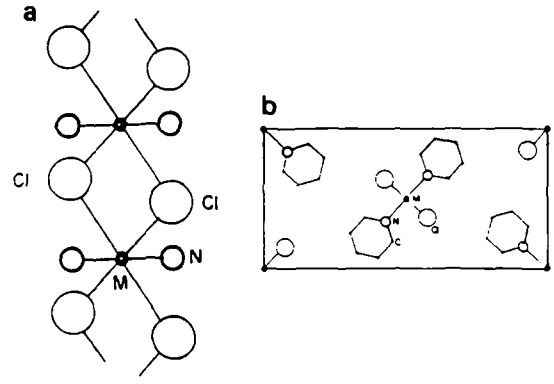

Fig. 3. (a) The schematical structure of the $-MCl_2-$chain in the *ac* plane (see for details Ref. [16]); M means "metal" (for example, M ≡ Co); (b) the rough sketch of $MCl_2 \cdot 2NC_5H_5$ structure viewed down along the *c*-axis.

3. Magnetic Ising systems

Before proceeding with consideration of information transfer in alternating Ising spin systems, we briefly review the physical parameters of real one-dimensional Ising systems, mainly following Refs. [14,15]. As an example we shall consider here only magnetic systems. There are many substances in which real localized spins of paramagnetic atoms organize themselves into linear chains. In fact, this occurs whenever the exchange interaction J between spins in a chain is much larger than the interchain exchange interaction J'. Of course, such systems are actually three-dimensional. In these systems a magnetic ordering takes place at sufficiently low temperatures $T_c \sim J'$. At intermediate temperatures $J > T > T_c$ these systems are in the paramagnetic state, and their thermodynamical properties are determined by their one-dimensional correlations. In what follows, the signs of the values J and J' are not important for us, as the main interaction in our case is the Zeeman interaction of the ionic spins with an external dc magnetic field H. Often the reason that such one-dimensional chains appear is connected with the presence of non-magnetic ions or complexes that separate different chains. As a well-known example of a one-dimensional system, in Fig. 3 the structure of $MCl_2 \cdot 2NC_5H_5$ [16] is shown, where M means "metal".

We present, as examples, five substances whose thermodynamic properties may be successfully described by the one-dimensional Ising Hamiltonian with different values J [13,14,16–18],

$$CoCl_2 \cdot 2H_2O, \quad J = 18\ \mathrm{K},$$
$$CoCl_2 \cdot 2NC_5H_5, \quad J = 9.5\ \mathrm{K},$$
$$K_3Fe(CN)_6, \quad J = -0.23\ \mathrm{K},$$
$$(NH_4)_2MnF_5, \quad J = -12\ \mathrm{K},$$
$$RbFeCl_3 \cdot 2H_2O, \quad J = -35\ \mathrm{K}. \tag{3.1}$$

The question arises, whether the resonant properties of real Ising systems could be described as a local inversion of spins. The answer is positive. In Refs. [17,18] the infra-red transmission was studied in $CoCl_2 \cdot 2H_2O$ at liquid helium temperatures, and at magnetic field up to 6 T. The authors of Refs. [17,18] observed the local inversion of clusters consisting of up to 14 adjacent spins, in the frequency region ~ 30 cm^{-1} ($\sim 10^{12}$ Hz). When the external magnetic field vanishes, $H = 0$, all these excitations have the same frequencies. But for $H \neq 0$ the energy of each excitation grows linearly with the cluster size. In Ref. [20] the authors studied the same crystal at liquid helium temperature, and with magnetic field ~ 5 T, but in another frequency region 20–50 GHz (i.e. ~ 1 cm^{-1}). They observed resonant transitions connected with either increasing, or decreasing of the size of the thermal clusters in a dc magnetic field (see Fig. 4). As in the usual magnetic resonance experiments, the magnetic quantum number m changes in experiments [20] by unity ($m \to m \pm 1$), and the frequency of res-

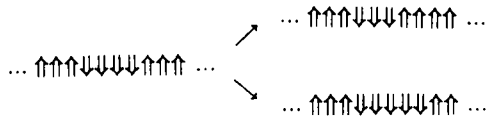

Fig. 4. Increasing and decreasing of the cluster size in the experiment [20].

onance is equal to γH, where γ is the gyromagnetic ratio of spins.

As far as we are aware, Ising systems have been experimentally investigated in detail only for homogeneous chains, for which $\omega_i=\omega$ and $J_i=J$. The first step in realizing an Ising quantum computer is to create an appropriate Ising chain with two inequivalent spins AB AB.... We believe that such binary Ising chains could be realized experimentally. There is a relatively new class of one-dimensional materials in which two different spins alternate regularly along a chain [21] with either different metal ions, or a metal ion and a radical. The purpose in creating systems of this kind is mainly connected with designing a bulk molecular ferromagnet. In this connection we mention, for example, the ordered binary chain compound, $CuMnC_7H_{12}N_2O_{10}$, with alternating Mn ($S=\frac{5}{2}$) and Cu ($S=\frac{1}{2}$) ions [22]. These single crystals were obtained by slow diffusion of two solutions containing Cu and Mn ions over about three months. The structure of the bimetallic chain is shown in Ref. [22]. In this crystal one has the so-called "oxamato bridges" between the adjacent Mn and Cu ions. These bridges provide strong antiferromagnetic interaction in spite of the large separation between ions.

We want to emphasize that for our purposes of quantum computations it is important to have two alternating g-factors. It is clear that the same ions in alternating surroundings can have different resonance frequencies, and vice versa, different ions can have the same frequencies.

Next, we consider the situation for a binary Ising chain with two different frequencies ω^{A} and ω^{B}. The interaction splits each of these frequencies into three,

$$\omega^{\mathrm{A}}_{00}=\omega^{\mathrm{A}}+2J\,,\quad \omega^{\mathrm{A}}_{01}=\omega^{\mathrm{A}}_{10}=\omega^{\mathrm{A}}\,,$$
$$\omega^{\mathrm{A}}_{11}=\omega^{\mathrm{A}}-2J\,. \tag{3.2}$$

Analogous expressions exist for ω^{B}_{ik}. We suppose, for example, that $\omega^{\mathrm{A}}>\omega^{\mathrm{B}}$, and the difference $\omega^{\mathrm{A}}-\omega^{\mathrm{B}}$ is about or exceeds $6J$. We suggest using this kind of chain in experiments for quantum computations. For this application, the first problem is a thorough analysis of the technology of creating "binary Ising systems" (BIS): AB AB.... .

The parameters of a BIS magnetic Ising system must be restricted in order to be a viable candidate for quantum computations. In particular, the following inequalities should be satisfied,

$$kT\ll g\mu H\,,\quad g\mu\Delta H\ll J\ll g\mu H\,, \tag{3.3}$$

where $\mu\equiv\mu_{\mathrm{B}}=e/2mc$ is the Bohr magneton, $g\mu\Delta H$ is the width of the line, and $g\mu=\hbar\gamma$. (The value of g for a free electron is $g=2$, but in the crystal field g can differ from this value.) The condition $kT\ll g\mu H$ allows the unexcited spins to be in the ground state. The condition $g\mu\Delta H\ll J$ means that the width of the energy-level lines is small in comparison with the splitting of levels. Finally, the condition $J\ll\mu H$ provides the small parameter for weak spin–spin interaction in the system.

For example, we may take

$$T\sim 1\,\mathrm{K}\,,\quad H\sim 10\,\mathrm{T}\,,\quad \Delta H\sim 10^{-1}\,\mathrm{T}\,,\quad J\sim 1\,\mathrm{K}\,. \tag{3.4}$$

We note that the usual quantity ΔH in electronic paramagnetic resonance is of the order 10^{-4}–10^{-2} T [23]. It may appear that the design of a quantum computer based on one-dimensional Ising systems requires abnormally low temperature, or high magnetic field strength, for device operation. Our opinion is that such conditions are justifiable, for addressing fundamental research problems in quantum computation rather than for immediate application.

Also we note that standard experimental investigations of magnetic Ising systems typically use substances with high values of J ($J>kT$). It is important to note that for the above quantum computer considerations the condition $J>kT$ is not obligatory. Indeed, because the resonant frequency is determined by the external magnetic field H, we only need the condition $J\gg g\mu\Delta H$. An important remaining problem is to investigate the resonant and the relaxation properties of binary Ising systems that are appropriate candidates for quantum computer devices.

4. Loading and reading-out information

It is clear the BISs can be used for loading information. For this purpose we can use, for example, the

sequence of pulses (1.1) suggested in Ref. [11]. To read-out the information one can use the sequence of two π-pulses suggested in Ref. [13]. It may be more convenient in experiments to read-out the information using a $\pi/2$ pulse. For example, let us consider the edge spin, assuming, say, that it is a B spin. To read-out the information we can move the bit that we want to read-out to the spin A that is a neighbor to the edge spin. If spin A is in the excited state, then the frequency of the edge spin is $\omega_1^B = \omega^B - J$. To read-out the information one can apply $\pi/2$ pulse with a carrier frequency of $\omega^B - J$. If one detects the photon signal of free precession, one can conclude that the atom A is in the excited state. After detecting a signal one can apply an additional $\pi/2$ pulse of the opposite phase to return the edge spin to the ground state. As in the scheme described in Ref. [11], use of this scheme requires several copies of the chains, in order to detect the signal reliably.

It is known that the estimation of the maximum sensitivity in electron paramagnetic spin resonance at normal conditions ($T \sim 4$ K and $H \sim 0.3$ T) allows detection of a signal from 10^5 spins [24]. According to Ref. [24], when the external magnetic field grows, this number decreases as H^{-2} until the condition $kT > g\mu H$ is satisfied. Consequently, we expect that the number of copies required to read-out the information in the Ising systems considered here will be mainly determined by the diameter of a laser beam.

We note that in principle one could use a π pulse rather than a $\pi/2$ pulse and detect a signal due to this pulse. Although this approach would not be convenient for real experiments, it does show that the process of reading-out may be organized as a reversible process.

BISs could also be used for information processing. For example, let us consider the BIS system ABA... with the edge spin A. Applying to this system the sequence of π pulses

$$\omega_1^A \omega_{11}^B \omega_1^A , \tag{4.1}$$

provides an exchange of bits between the first two spins A and B if and only if the third spin A is in the excited state. This is the BIS Fredkin gate with the third spin A as the control unit. Such a BIS Fredkin gate could be used as one of the simplest quantum logical devices. Consider the following simple experiment with the BIS Fredkin gate. Let the initial state of the whole BIS system be the ground state. We apply a pulse with frequency $\omega_0^A = \omega^A + J$. This pulse excites the edge spin A (the first spin). Then, we apply pulses with frequencies $\omega_{10}^B \omega_{10}^A$ which excite the second and the third spins. After these sequences of pulses, the first three spins are in their excited states. Now we derive the edge spin A into the ground state. For this, one applies a pulse with frequency ω_1^A. To realize the open BIS Fredkin gate, we apply the sequence (3.9) which changes the states of the two first spins A and B because the third spin A is in the excited state. Finally, to read-out the information from the second spin B we apply a $\pi/2$ pulse with frequency ω_0^A. As the result, after this pulse we should observe the signal of free precession. Analogously, we can realize this experiment with a closed BIS Fredkin gate. For this, we use the same pulses except we omit the pulse with frequency ω_{10}^A. In this case the signal of free precession will not be observed.

Finally, we estimate the pulse parameters required in the scheme just discussed. For $H \sim 10$ T, the resonant frequency is about 300 GHz (~ 10 cm^{-1}). In such experiments one can use quasi-optical techniques in the far-infrared spectrum [25]. Suppose that the pulse duration τ is about 10 ns. Then, for the π-pulse one needs the amplitude of the alternating field to be $h \sim 1.5$ mT. For the "normal" action of a π-pulse (i.e. to populate the upper state close to 100%) there is an additional restriction on ΔH,

$$\Delta H \ll h . \tag{4.2}$$

One can take $\Delta H \sim 10^{-4}$ T, which is still reasonable for electronic paramagnetic resonance. Finally, the time of the longitudinal relaxation T_1 should be longer than both the pulse duration and the time between pulses τ' (we may take $\tau' \sim 10$ ns, as well). The wide distribution of the quantity T_1 for 3D ions at liquid helium temperature, from 10 μs to 1 s [25,26], allows this scheme to be feasible, in principle, as a research task.

5. Conclusion

Alternating Ising systems in the parameter regime discussed here of possible use for quantum computer operations lie in an interesting, as yet sparsely studied domain of condensed matter physics. There are

many questions as yet unaddressed in this quasi-optical domain of spin dynamics in the presence of high magnetic fields. Moreover, to design a quantum computer using the BIS type of Ising system discussed here, at least the following problems should be addressed.

(1) Complete an analysis of the existing Ising systems, both magnetic and non-magnetic, and choose the most appropriate class of such systems;

(2) Analyze the technology for creating Ising systems to choose a method of designing the proper BISs;

(3) Perform theoretical, computational and experimental analysis of resonant and relaxation properties of BISs;

(4) Perform numerical and real experiments for loading, processing and reading-out information on BISs;

(5) Analyze more complicated alternating Ising systems than BISs, as necessary.

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